2-(P-nonylphenoxy)-6-benzyl pyrazine

Inchi: InChI=1S/C26H32N2O/c1-2-3-4-5-6-7-9-12-22-15-17-25(18-16-22)29-26-21-27-20-24(28
InchiKey: PJHZIBWEHBLJKC-UHFFFAOYSA-N
Formula: C26H32N2O
SMILES: CCCCCCCCCc1ccc(Oc2cncc(Cc3ccccc3)n2)cc1
Mol. weight [g/mol]: 388.55
CAS: 116295-69-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.47		Crippen Method
logp	7.153		Crippen Method
mcvol	331.750	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C116295693&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume